

Theory and Simulation of Nano Scale Materials

CINT, Albuquerque, New Mexico

October 14-15, 2010

Thursday October 14 AM Reactions at Surfaces & Interfaces

8:30-8:40am Welcome – CINT Director

Chairs: Stephen Gray, Normand Modine

8:40-9:20am Peter J. Feibelman (Sandia National Laboratories)

- How water binds to precious metal surfaces

9:20-9:45am Mark Hybertsen (Brookhaven National Laboratory)

- Exploring novel materials for photocatalytic water splitting

9:45-10:10am Jeffrey Greeley (Argonne National Laboratory)

- Ab-initio simulations of anocatalysis and corrosion

10:10-10:25am Break

10:25-10:50am Larry Curtiss (Argonne National Laboratory)

- Density functional studies of the reactivity of supported metal nanoclusters

10:50-11:20am Ping Liu (Brookhaven National Laboratory)

- Theoretical insight into the water-gas shift catalysts

11:20-11:50am Stephen Gray (Argonne National Laboratory)

- Size-dependent chemical effects in the spectroscopy of metallic nanoparticles

11:50-12:15 Subramanian Sankaranarayanan (Argonne National Laboratory)

- Atomistic simulations of oxidation and ultra-thin oxide growth on metal and metal alloys

Lunch

Thursday October 14 PM Charge and Energy Transport and Conversion

Chair: Bobby Sumpter

1:45-2:10pm pm Norman Modine (Sandia National Laboratories)
- Coupled Ionic and Electronic Heat Transport at the Nanoscale

2:10-2:35pm Jingsong Huang (Oak Ridge National Laboratories)
- Modeling capacitive energy storage in carbon nanosystems

2:35-3:00pm Sergei Tretiak (Los Alamos National Laboratory)
- Modeling of Non-adiabatic Photoinduced Dynamics for Photovoltaic Applications

3:00-3:25pm Alexander V. Balatsky (Los Alamos National Laboratories)
- Dirac materials and nanoscale defects

3:25-3:50pm Barry Farmer (Air Force Research Laboratory)
- Role for Computational Tools in the Future of Materials Research and Utilization

3:50-4:15 pm Break

4:15-5:30pm Poster Session

Thursday Dinner – 7:00pm - Artichoke Cafe

Friday October 15 AM Soft and Bio Nanomaterials and Nanoscale Self-Assembly

Chairs: Gary Grest, Mark Stevens

8:30-8:55am Miguel Fuentes-Cabrera (Oak Ridge National Laboratories)
- Unnatural DNAs: from nanotechnology to prebiotic chemistry; and back

8:55-9:20am Mark Stevens (Sandia National Laboratories)
- Neurofilaments as a charged polymer brush

9:20-9:45am Steve Whitelam (Lawrence Berkeley National Laboratory)
- Nonclassical assembly pathways of anisotropic particles

9:45-10:10am Bobby Sumpter (Oak Ridge National Laboratory)
- Nanoscale self-assembly and interfacial interactions

10:10-10:30am Break

10:30-10:55am Amalie Frischknecht (Sandia National Laboratories)

- Structure and phase behavior of soft nanomaterials from classical density functional theory

10:55-11:20am Alexei Tkachenko (Brookhaven National Laboratory)

- Nanoparticles with key-lock interactions: from mess to order and complexity

11:20-11:55am Gary Grest (Sandia National Laboratories)

- Coated nanoparticles in solution and at liquid/vapor interfaces

Lunch

Friday October 15 PM Methodology for the Nanoscale

Chairs: Mark Hybertsen, Glenn Martyna

1:30-1:55pm Ye Xu (Oak Ridge National Laboratory)

- Nano-scale size and environmental effects in the reactivity of platinum clusters

1:55-2:20pm Jeff Neaton (Lawrence Berkeley National Laboratory)

- First-principles studies of energy conversion at nanoscale interfaces

2:20-2:55pm David Prendergast (Lawrence Berkeley National Laboratory)

- Simulating core-level spectroscopy from first principles

2:55-3:20pm Paul Kent (Oak Ridge National Laboratory)

- New developments in electronic structure quantum Monte Carlo

3:20-3:40 Break

3:20-4:05pm Qin Wu (Brookhaven National Laboratory)

- Energy decomposition analysis: bridging quantum chemistry and classical force fields

4:05-4:30pm Gonzalo Alvarez (Oak Ridge National Laboratory)

- Collective Phenomena in Nanoscience: The Role of Diagonalization and Quantum Monte Carlo Solvers

4:30-4:55pm Stuart Trugman (Los Alamos National Laboratory)

- Quantum dynamics of electron-phonon coupling

Inquiries should be directed to the conference chair Gary Grest:

gsgrest@sandia.gov Phone: 505-844-3261